### ICGE Module 2 Session 4

#### Scientific application of Python: Random Walks



#### Left:

https://commons.wikimedia.org/wiki/File:Random\_walk\_25000.gif

#### Right:

http://www.mit.edu/~kardar/teaching/projects/chemotaxis(AndreaSchmidt)/finding\_food.htm

## Many problems in physics, chemistry and biology essentially boil down to "random walks"



Simplest question to ask—does the walker ever get back home?

### Python program for 1-D random walk

```
from _______ import division
from random import choice
trials=1000
steps=1000
gothome=0
for i in range(trials):
    point=0
    for step in range(steps):
        point+=choice((-1,1))
        if point==0:
            gothome+=1
            break
print "Fraction that got home=%f" % (gothome/trials)
```

Save this as "rwalk1d.py" and run for different numbers of steps

## The problem gets more interesting if the walker moves in 2 or more dimensions



Note that if we randomly change both x & y coordinates by -1 or +1, the walker moves diagonally like a checkers piece.

### Python program for arbitrary-D random walk making diagonal moves at every step

```
from ______ import division
from random import choice
dim=3
trials=1000
steps=1000
gothome=0
for i in range(trials):
    point=[0]*dim
    for step in range(steps):
        for j in range(dim):
            point[j]+=choice((-1,1))
        if point.count(0)==dim:
            gothome+=1
            break
print "Fract that got home=%f in %d dims" % (gothome/trials,dim)
```

Save this as "rwalknd.py" and run for different dimensions

For what #'s of dimensions does the walker make it home?

# Exact results for an infinite number of steps moving in only one dimension at a time

Prob(get home)
1.000
1.000
0.341
0.193
0.135
0.105
0.086
0.073

(2,-2)	(2,-1)	(2,0)	(1,1)	(2,2)
(1,-2)	(1,-1)	(1,0)	(1,1)	(1,2)
(0,-2)	(0,-1)	<b>於</b> (0,0)	(0,1)	(0,2)
(-1,-2)	(-1,-1)	(-1,0)	(1,1)	2,2)
(-2,-2)	(-2,-1)	(-2,0)	-2,1)	(-2,2)

Research questions:

- 1. How well does rwalknd.py agree with the exact results?
- 2. Do your results match better if you modify the program to step in only one dimension at a time?

Exact results from http://mathworld.wolfram.com/PolyasRandomWalkConstants.html

## Python program for arbitrary-D random moving in just one dimension each step

```
from ______ import division
from random import choice
dim=3
trials=1000
steps=1000
gothome=0
for i in range(trials):
    point=[0]*dim
    for step in range(steps):
        movedim=choice(range(dim))
        point[movedim]+=choice((-1,1))
        if point.count(0)==dim:
            gothome+=1
            break
print "Fract that got home=%f in %d dims" % (gothome/trials,dim)
```

Save this as "rwalknd2.py" and run for different dimensions

Do these results agree better with pure theory?

# Another important type of random walk simulation is diffusion-limited aggregation (DLA)

DLA "crystal" in copper sulfate solution



We can simulate DLA with a random 2-D walk where the particle stops if it hits an existing particle



https://en.wikipedia.org/wiki/Diffusion-limited\_aggregation

## DLA Python program using very simple graphics based on the Python Image Library (PIL)

```
from random import choice
from drawgridlib import drawgrid, savegrid
npart=200 #Number of particles to aggregate
side=75 #Should be an odd number
steps = [(1,0), (-1,0), (0,1), (0,-1)]
grid=[[0 for x in range(side)] for y in range(side)]
grid[side/2][side/2]=1
for ipart in range(npart):
    # Start particle at origin
    x,y = 0,0
    # perform the random walk until particle aggregates
    while 1:
        grid[x][y]=0 #Remove particle from current spot
        # Randomly move particle
        sx,sy = choice(steps)
        x += sx
        y += sy
        # Enforce periodic boundaries
        if x < 0: x = side - 1
        if y < 0: y=side-1
        if x==side: x=0
        if y==side: y=0
        grid[x][y]=1 #Put particle in new location
        # Stop if you are next to a particle
        if (grid[(x+1)%side][y]+grid[x][(y+1)%side]+
            grid[(x+side-1)%side][y]+grid[x][(y+side-1)%side])>0:
            break
drawgrid(grid, side) #Displays image to screen
#savegrid(grid,side) #Stores image in dla.jpg
```

#### Simulation grid



Output

